

## Probing Hydrogen Bonding in Water and Ice using X-rays.

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In many processes in technology and nature, hydrogen bonding (H-bonding) is involved as an essential component. The H-bond in liquid water holds the key to its peculiar behavior, with implications for chemical, biological and geological processes. In the present talk I will show how we can address the nature of the H-bond and its connection to the structure of liquid water using a combination of X-ray spectroscopy and Density Functional Theory (DFT) calculations. X-ray Absorption Spectroscopy (XAS), X-ray Emission Spectroscopy (XES) and X-ray Raman Scattering (XRS) provides direct information on how occupied and unoccupied orbitals locally around the oxygen atom are transformed upon condensation of water to form ice, ambient water, supercritical water and water adsorbed on surfaces. In particular the recent result on the structure of the first coordination shell in liquid water (1) challenges many current models based on molecular dynamic simulations.

1. Wernet et. al. , *Science* **304**, 995 (2004).